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EUCLIDEAN AND CIRCUM-EUCLIDEAN DISTANCE MATRICES: CHARACTERIZATIONS AND LINEAR PRESERVERS*

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Abstract. Short proofs are given to various characterizations of the (circum-)Euclidean squared distance matrices. Linear preserver problems related to these matrices are discussed.

Key words. Distance geometry, Multidimensional scaling, Eigenvalues, Interlacing inequalities, Linear preservers.

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1. Introduction. Distance geometry is concerned with the interpoint distances of configurations of n points in metric spaces, see [2]. It is natural to organize these interpoint distances in the form of an $n \times n$ *distance matrix*, so the study of distance geometry inevitably borrows tools from matrix theory.

Distance matrices have important applications in a variety of disciplines. Distance matrices were first introduced (anonymously) by A. Cayley [3] in 1841 to derive a necessary condition involving matrix determinants for five points to reside in Euclidean space. Nearly a century after Cayley's contribution, a characterization of distance matrices (re)discovered by G. Young and A.S. Householder [14] was the impetus for (classical) multidimensional scaling [6, 11, 13]. Originally developed by psychometricians and statisticians, multidimensional scaling is a widely used tool for data visualization and dimension reduction. Research on multidimensional scaling continues to exploit facts about distance matrices, e.g., [10]. Analogously, in computational chemistry and structural molecular biology, the problem of determining a

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molecule's 3-dimensional structure from information about its interatomic distances is the problem of finding a matrix of 3-dimensional Euclidean distances that satisfies certain constraints, as in [4].

It turns out that it is more convenient to encode the squares of the distances between the points, and define a *Euclidean (squared) distance* (ESD) matrix $A = (a_{ij})$ as a matrix for which there exists $x_1, \ldots, x_n \in \mathbb{R}^k$ such that $a_{ij} = \|x_i - x_j\|^2$ for a certain positive integer k. Let $\mathbf{S}_n$ denote the set of $n \times n$ symmetric matrices and let $\mathrm{ESD}(n)$ denote the subset of ESD matrices. Then $\mathrm{ESD}(n)$ is a convex cone in $\mathbf{S}_n$ with many intriguing properties.

In this paper, we study ESD matrices and *circum-Euclidean (squared) distance* (CESD) matrices, i.e., $A = (\|x_i - x_j\|^2)$ with $\|x_1\| = \cdots = \|x_n\|$. In Section 2, we provide short proofs (some new) of a number of well-known characterizations of ESD matrices. In Section 3, we give characterizations of (CESD) matrices. In Section 4, we characterize linear maps leaving invariant subsets of $\mathrm{ESD}(n)$ and $\mathrm{CESD}(n)$. This can be regarded as a special instance of the general research of linear preserver problems; see [9].

2. Characterizations. Characterizations of distance matrices are mathematically elegant, but also genuinely useful to researchers in other disciplines. In the following, we provide short proofs of several well-known characterizations of Euclidean (squared) distance matrices.

It follows immediately from the definition that an ESD matrix $A = (a_{ij})$ with $a_{ij} = \|x_i - x_j\|^2$, where $x_1, \ldots, x_k \in \mathbb{R}^k$, is a real, symmetric, nonnegative, hollow ($a_{ii} = 0$) matrix. These properties are necessary but not sufficient for a matrix to be an ESD matrix (a matrix with these properties is called a pre-distance or dissimilarity matrix). If k is the smallest dimension for which such a construction is possible, then k is the embedding dimension of A. Furthermore, the choice of $x_1, \ldots, x_n$ is not unique, for if $\tilde{x}_i = x_i - x_0$ then $\tilde{x}_i - \tilde{x}_j = x_i - x_j$. Given $w = (w_1, \ldots, w_n)^t \in \mathbb{R}^n$ with $\sum_{j=1}^n w_j \neq 0$, let $x_0 = \sum_{j=1}^n w_j x_j / \sum_{j=1}^n w_j$. Then $\sum_{j=1}^n w_j \tilde{x}_j = 0 \in \mathbb{R}^k$, so we can assume without loss of generality that $\sum_{j=1}^n w_j x_j = 0 \in \mathbb{R}^k$. For notation simplicity, we often assume that $\sum_{j=1}^n w_j = 1$.

Let $e_1, \ldots, e_n$ denote the coordinate unit vectors in $\mathbb{R}^n$ and let I denote the $n \times n$ identity matrix. Set $e = e_1 + \cdots + e_n$ and $J = ee^t$. Given $w \in \mathbb{R}^n$ such that $e^t w = 1$, define the linear mapping $\tau_w : \mathbf{S}_n \to \mathbf{S}_n$ by

$$\tau_w(A) = -\frac{1}{2}\left(I - ew^t\right) A \left(I - we^t\right).$$

Given $w \in \mathbb{R}^n$, we say that $x_1, \ldots, x_n \in \mathbb{R}^k$ is w-centered if and only if $\sum_{j=1}^n w_j x_j = 0$.

THEOREM 2.1. *Suppose that A is an $n \times n$ real, symmetric, hollow matrix. Let*

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w be any vector in $\mathbb{R}^n$ such that $e^tw = 1$ and let U be any $n \times (n-1)$ matrix for which the $n \times n$ matrix $V = (\frac{e}{\sqrt{n}}|U)$ is orthogonal. Then the following conditions are equivalent.

(a) *There exists a w-centered spanning set of $\mathbb{R}^k$, $\{x_1, \ldots, x_n\}$, for which $A = (\|x_i - x_j\|^2)$.*
(b) *There exists a w-centered spanning set of $\mathbb{R}^k$, $\{x_1, \ldots, x_n\}$, for which $\tau_w(A) = (x_i^t x_j)$.*
(c) *The matrix U^tAU is negative semidefinite of rank k.*
(d) *The submatrix B in*

$$\hat{A}_0 = \begin{pmatrix} 1 & 0 \\ 0 & V^t \end{pmatrix} \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & V \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & * & * \\ 0 & * & B \end{pmatrix}$$

is negative semidefinite of rank k.
(e) *The matrix $A_0 = \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix}$ has has one positive and $k+1$ negative eigenvalues.*
(f) *There is an $n \times n$ permutation matrix P for which the matrix $\begin{pmatrix} 0 & e^t \\ e & P^tAP \end{pmatrix}$ has rank $k+2$, and, for $j = 2, \ldots, k+2$, each $j \times j$ leading principal minor is nonzero and has sign $(-1)^{j-1}$.*

Proof. We first establish the equivalence of conditions (a), (b), and (c).

(c) $\Rightarrow$ (b). Let $v_1, \ldots, v_n$ denote the rows of V and let $u_1, \ldots, u_n$ denote the rows of U. It follows from

$$I = VV^t = \begin{pmatrix} \frac{e}{\sqrt{n}} & U \end{pmatrix} \begin{pmatrix} e^t/\sqrt{n} \\ U^t \end{pmatrix} = \frac{1}{n}J + UU^t$$

that $UU^t = I - \frac{1}{n}J$. Hence, it follows from $Jwe^t = ee^twe^t = ee^t = J$ that

$$UU^t\left(I - we^t\right) = \left(I - \frac{1}{n}J\right)\left(I - we^t\right) = \left(I - we^t\right) - \frac{1}{n}(J - J) = \left(I - we^t\right).$$

Because U^tAU is a negative semidefinite matrix of rank k, we can find some $k \times (n-1)$ matrix Y of rank k such that $-\frac{1}{2}U^tAU = Y^tY$. Let $W = U^t(I - we^t)$ and let $x_1, \ldots, x_n$ denote the columns of $X = YW$. Then

$$\sum_{j=1}^{n} w_j x_j = Xw = YU^t\left(I - we^t\right)w = YU^t(w - w) = 0$$

and

$$X^tX = W^tY^tYW = -\frac{1}{2}W^tU^tAUW = -\frac{1}{2}\left(I - we^t\right)^t UU^tAUU^t\left(I - we^t\right)$$

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$$= -\frac{1}{2}\left(I - ew^t\right) A \left(I - we^t\right) = \tau_w(A).$$

It remains to show that $x_1, \ldots, x_n$ spans $\mathbb{R}^k$. The range space of U is $e^\perp$. If $z \in e^\perp$, then

$$\left(I - we^t\right) z = z; \tag{2.1}$$

hence, U^t and $U^t(I - we^t)$ have the same range space. Furthermore, because $YU^t = (0|Y)V^t$, rank $YU^t =$ rank $Y = k$. Hence,

$$\text{rank } X = \text{rank } YW = \text{rank } YU^t \left(I - we^t\right) = \text{rank } YU^t = k.$$

(b) ⇒ (a). Define $\kappa : \mathbf{S}_n \to \mathbf{S}_n$ by

$$\kappa(B) = \text{diag}(B)J - 2B + J\text{diag}(B).$$

Let $X = (x_1|\cdots|x_n)$ and

$$H = \kappa\left(X^tX\right) = \left(x_i^tx_i - 2x_i^tx_j + x_j^tx_j\right) = \left(\|x_i - x_j\|^2\right). \tag{2.2}$$

Because $J(I - we^t) = J - J = 0$ and $X(I - we^t) = X - Xwe^t = X$,

$$\tau_w(H) = -\frac{1}{2}\left(I - ew^t\right)\left(DJ - 2X^tX + JD\right)\left(I - we^t\right) = X^tX = \tau_w(A).$$

Furthermore, it follows from (2.1) that

$$\left(I - we^t\right)(e_i - e_j) = e_i - e_j,$$

so

$$\begin{aligned} H_{ij} &= -\frac{1}{2}(e_i - e_j)^t H (e_i - e_j) = (e_i - e_j)^t \tau_w(H)(e_i - e_j) \\ &= (e_i - e_j)^t \tau_w(A)(e_i - e_j) = A_{ij}, \end{aligned}$$

i.e., $H = A$.

Notice that this argument demonstrates that τ_w is injective on the hollow symmetric matrices.

(a) ⇒ (c). Let $x_0 = \sum_{j=1}^n x_j/n$ and $\tilde{x}_i = x_i - x_0$, so that $\tilde{x}_1, \ldots, \tilde{x}_n$ is an e-centered spanning set of $\mathbb{R}^k$ with $A = (\|\tilde{x}_i - \tilde{x}_j\|^2)$. Let $\tilde{X}$ denote the $k \times n$ matrix with columns $\tilde{x}_1, \ldots, \tilde{x}_n$. Then $\tilde{X}e = 0$, so $\tilde{X}V = (0|\tilde{X}U)$ and it follows that rank $\tilde{X}U =$ rank $\tilde{X} = k$.

Because V is orthogonal, $U^te = 0$ and therefore $U^tJ = U^tee^t = 0 = JU$. Applying (2.2),

$$U^tAU = U^t\left(JD - 2\tilde{X}^t\tilde{X} + DJ\right)U = -2U^t\tilde{X}^t\tilde{X}U = -2\left(\tilde{X}U\right)^t\left(\tilde{X}U\right)$$

is a negative semidefinite matrix of rank k.

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(c) ⇔ (d). Because $U^te = 0$,

$$\hat{A}_0 = \begin{pmatrix} 1 & 0 \\ 0 & V^t \end{pmatrix} \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & V \end{pmatrix} = V_0^t A_0 V_0$$
$$= \begin{pmatrix} 1 & 0 \\ 0 & e^t/\sqrt{n} \\ 0 & U^t \end{pmatrix} \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & e/\sqrt{n} & U \end{pmatrix}$$
$$= \begin{pmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & e^tAe/n & * \\ 0 & * & U^tAU \end{pmatrix}. \tag{2.3}$$

Thus, $B = U^tAU$ and conditions (c) and (d) are equivalent.

Now we establish the equivalence of conditions (d), (e), and (f).

(d) ⇒ (e). Because V is orthogonal, so is V_0 and it follows from (2.3) that A_0 and $\hat{A}_0$ have the same eigenvalues. By interchanging the first two rows of $\hat{A}_0$ and performing Gaussian elimination, we see that rank A_0 = rank $\hat{A}_0 = 2+$rank $B = 2+k$. Because $\begin{pmatrix} 0 & 0 \\ 0 & B \end{pmatrix}$ has no positive eigenvalues and is a principal submatrix of $\hat{A}_0$, it follows from the interlacing inequalities that $\hat{A}_0$, hence A_0, has at most one positive eigenvalue. But the leading 2×2 principal submatrix of A_0 has a negative determinant and therefore one positive and one negative eigenvalue; hence, by the interlacing inequalities, A_0 has at least one positive eigenvalue. Thus, A_0 has exactly one positive eigenvalue and, because rank $A_0 = k+2$, $k+1$ negative eigenvalues.

(e) ⇒ (d). We have already argued that rank B = rank $\hat{A}_0 - 2$ = rank $A_0 - 2 = k+2-2 = k$. Given $v \in \mathbb{R}^{n-1}$, we demonstrate that $b = v^tBv \leq 0$. Toward that end, let

$$D = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & v^t \end{pmatrix} \hat{A}_0 \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & v \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & c & * \\ 0 & * & b \end{pmatrix},$$

where $c = e^tAe/n$. Notice that $\det(D) = -nb$.

Let $d_1 \geq d_2 \geq d_3$ denote the eigenvalues of D. Let Q be any orthogonal matrix of the form

$$Q = \left(\begin{array}{ccc|c} 0 & 1 & 0 & \\ 1 & 0 & 0 & * \\ 0 & 0 & v & \end{array} \right),$$

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in which case $Q^t\hat{A}_0Q = \begin{pmatrix} D & * \\ * & * \end{pmatrix}$ has the same eigenvalues as $\hat{A}_0$, i.e., the same eigenvalues as A_0. Because D is a principal submatrix of $Q^t\hat{A}_0Q$, it follows from the interlacing inequalities that $d_3 \leq d_2 \leq 0$. Furthermore, it follows from the Rayleigh-Ritz Theorem that $d_1 \geq 0$. We conclude that $b = -\det(D)/n = -d_1d_2d_3/n \leq 0$.

(e) ⇒ (f). Any matrix of the form

$$\begin{pmatrix} 0 & e^t \\ e & P^tAP \end{pmatrix}, \tag{2.4}$$

where P is an $n \times n$ permutation matrix, must have the same eigenvalues as A_0. It follows from (e) that any such matrix must have rank $k+2$. We choose P so that, for $j = 2, \ldots, k+2$, the $j \times j$ leading principal submatrices of (2.4) have no zero eigenvalues. Then the 2×2 leading principal submatrix is $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, which has a positive eigenvalue. Hence, for $j = 2, \ldots, k+2$, each $j \times j$ leading principal submatrix will have one positive and $j-1$ negative eigenvalues and the corresponding minors will have signs $(-1)^{j-1}$.

(f) ⇒ (e). Because (2.4) has rank $k+2$, so does A_0. Because the 2×2 leading principal minor of (2.4) is negative, the 2×2 leading principal submatrix has one positive and one negative eigenvalue. Because the 3×3 leading principal minor of (2.4) is positive, it follows from the interlacing inequalities that the 3×3 leading principal submatrix has one positive and two negative eigenvalues. Continuing in this manner, we conclude that the $(k+2) \times (k+2)$ leading principal submatrix, hence (2.4), hence A_0, has one positive and $k+1$ negative eigenvalues. □

Let us make some remarks about the characterizations established in Theorem 2.1. We have already noted that the requirement that $x_1, \ldots, x_n$ is w-centered entails no loss of generality; hence, condition (a) is simply the definition of a k-dimensional ESD matrix, i.e., an ESD matrix with embedding dimension k. Historically, condition (f) was the first alternate characterization discovered. Condition (b) is useful in finding a set of points satisfying the distance matrix. Theoretically, condition (c) is most useful. In the literature, it is sometimes stated slightly differently.

Remark 2.2. In Theorem 2.1, the statement in condition (c) that U^tAU is negative semi-definite can be restated as $\sum_{i,j=1}^{n} a_{ij}y_iy_j \leq 0$ whenever $\sum_{i=1}^n y_i = 0$, with equality whenever y is in some $n-1-k$-dimensional subspace of $e^{\perp}$.

Proof. Note that $e^ty = \sum_{i=1}^n y_i = 0$ is equivalent to $y = Ux$ for some $x \in \mathbb{R}^{n-1}$. Hence $\sum_{i,j=1}^n a_{ij}y_iy_j = y^tAy = x^tU^tAUx \leq 0$ exactly when U^tAU is negative semi-definite. Note that we can replace the inequality with an equality exactly when x is in

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the $n-1-k$-dimensional null space of U^tAU, hence y is in some $n-1-k$-dimensional subspace of $e^\perp$. □

Using either statement for condition (c), we see that $\mathrm{ESD}(n)$ is a convex cone in $\mathbf{S}_n$, with embedding dimension increasing up to n. It is not easy to check this only using the definition of ESD matrices. Also, from conditions (c) and (e), we can easily deduce the possible ranks of an ESD matrix.

COROLLARY 2.3 (Gower [7]). *If $A \in \mathrm{ESD}(n)$ has embedding dimension k, then $\mathrm{rank}(A)$ equals $k+1$ or $k+2$.*

Proof. It follows from Theorem 2.1 (c) that U^tAU has k negative eigenvalues. Because U^tAU is a submatrix of V^tAV, it follows from the interlacing inequalities that V^tAV, hence A, has at least k negative eigenvalues. Furthermore, because $\mathrm{trace}(A) = 0$, A has at least one positive eigenvalue. Hence, $\mathrm{rank}(A)$ is at least $k+1$. Finally, it follows from (e) that $\mathrm{rank}(A_0) = k+2$. Because A is a submatrix of A_0, $\mathrm{rank}(A)$ is at most $k+2$. □

Gower [7, Theorem 6] distinguished between these two possible cases by demonstrating that $\mathrm{rank}(A) = k+1$ if and only if the points that generate A lie on a sphere. We will give a proof of this fact and some related results in the next section.

3. Circum-Euclidean squared distance matrices. A matrix $A \in ESD(n)$ is CESD if $A = (\|x_i - x_j\|^2)$ such that all $\|x_1\| = \cdots = \|x_n\|$. Recall that C is a correlation matrix if C is a positive semidefinite matrix with all diagonal entries equal to one. We have the following characterization of CESD matrices, and the minimum r such that $A = (\|x_i - x_j\|^2)$ with $r = \|x_1\| = \cdots = \|x_n\|$. Its proof depends heavily on the canonical form of A in (c).

THEOREM 3.1. *Suppose that $A \in \mathrm{ESD}(n)$ has embedding dimension k. Then the following are equivalent:*

(a) *A is a CESD matrix.*
(b) *There exist $\lambda \geq 0$ and a correlation matrix C such that $A = \lambda(ee^t - C)$, equivalently, $\lambda ee^t - A$ is positive definite.*
(c) *The intersection of the null space of $\left(I - \frac{J}{n}\right) A \left(I - \frac{J}{n}\right)$ and the range space of A has dimension one.*
(d) *Let $V = (\frac{e}{\sqrt{n}}|U)$ be an orthogonal matrix and*

$$V^tAV = \begin{pmatrix} \mathrm{tr}\, B & v^t \\ v & -B \end{pmatrix}.$$

Then there exists a vector $z \in \mathbb{R}^{n-1}$ such that $v = Bz$, i.e., v lies in the column space of B.
(e) $\mathrm{rank}(A) = k+1$.

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(f) $\sup\{w^tAw : e^tw = 1\} < \infty$.
(g) *There is* $w \in \mathbb{R}^n$ *and* $\beta \in \mathbb{R}$ *with* $e^tw = 1$ *such that* $Aw = \beta e$.
(h) *Let* $V = (\frac{e}{\sqrt{n}}|U)$ *be an orthogonal matrix such that*

$$(3.1) \qquad V^tAV = \left(\begin{array}{c|ccc|ccc} b_0 & b_1 & \cdots & b_k & b_{k+1} & \cdots & b_{n-1} \\ \hline b_1 & -\lambda_1 & & & & & \\ \vdots & & \ddots & & & 0 & \\ b_k & & & -\lambda_k & & & \\ \hline b_{k+1} & & & & & & \\ \vdots & & 0 & & & 0 & \\ b_{n-1} & & & & & & \end{array}\right),$$

$b_0 = \sum_{j=1}^k \lambda_j$. *Then* $b_{k+1} = \cdots = b_{n-1} = 0$.
(i) *There exists an* M *such that* $\sum\limits_{i,j=1}^{n} a_{ij}y_iy_j \le M \left(\sum\limits_{i=1}^{n} x_i\right)^2$ *for all* $y \in \mathbb{R}^n$.

Moreover, if these equivalent conditions hold and if $A = (\|x_i - x_j\|^2)$ *with* $r = \|x_1\| = \cdots = \|x_n\|$, *then*

$$2nr^2 \ge \operatorname{tr} B + (v^tB^{-1}v)^{1/2} = \left(b_0 + \sum_{j=1}^{k} b_k^2/\lambda_j\right)/n,$$

where B *is the matrix in condition (d), and* $b_0, b_1, \ldots, b_k, \lambda_1, \ldots, \lambda_j$ *are the quantities in (c).*

Proof. We prove the equivalence of these all but the last statement by pairs.

(a) $\Leftrightarrow$ *(b).* If $A = (\|x_i - x_j\|^2)$ such that $r = \|x_1\| = \cdots = \|x_n\|$, then

$$A = (\|x_i\|^2 + \|x_j\|^2 - 2x_i^tx_j) = \lambda(ee^t - C),$$

where $\lambda = 2r^2$ and $C = (x_i^tx_j)/r^2$ is a correlation matrix.

Conversely, if $A = \lambda(ee^t - C)$, where C is a correlation matrix. Then $C = (y_i^ty_j)$ for some unit vectors $y_1, \ldots, y_n$. Let $x_i = \sqrt{\lambda/2}y_i$ for $i = 1, \ldots, n$. Then $A = (\|x_i - x_j\|^2)$.

(b) $\Leftrightarrow$ *(h).* Suppose V is such that V^tAV has the form (3.1). Because $\Lambda = U^tAU$ is negative semidefinite of rank k, $\lambda_1, \ldots, \lambda_k > 0$.

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Suppose (b) holds. Writing $C = ee^t - A/\lambda$, it follows from (3.1) that

$$V^tCV = \frac{1}{\lambda}\left(\begin{array}{c|ccc|ccc} n\lambda - b_0 & -b_1 & \cdots & -b_k & -b_{k+1} & \cdots & -b_{n-1} \\ \hline -b_1 & \lambda_1 & & & & & \\ \vdots & & \ddots & & & 0 & \\ -b_k & & & \lambda_k & & & \\ \hline -b_{k+1} & & & & & & \\ \vdots & & 0 & & & 0 & \\ -b_{n-1} & & & & & & \end{array}\right). \tag{3.2}$$

Because λC, hence V^tCV, is positive semidefinite, so are the principal submatrices

$$\begin{pmatrix} n\lambda - b_0 & -b_i \\ -b_i & 0 \end{pmatrix},$$

which necessitates $b_i = 0$ for $i = k+1, \ldots, n-1$.

Conversely, suppose $b_{k+1} = \cdots = b_{n-1} = 0$. Then the matrix V^tCV in (3.2) is positive semidefinite if and only if S^tV^tCVS is positive definite where S is an invertible matrix. In particular, let $S = D^{-1}P$ where $D = \text{diag}(1, \sqrt{\lambda_1}, \ldots, \sqrt{\lambda_k}, 1, \ldots, 1)$ and P is an orthogonal matrix so that the first two rows of P^t are

$$(1, 0, \ldots, 0) \quad \text{and} \quad \frac{1}{\gamma}\left(0, \frac{b_1}{\sqrt{\lambda_1}}, \ldots, \frac{b_k}{\sqrt{\lambda_k}}, 0, \ldots, 0\right),$$

respectively, where $\gamma = \left\{\sum_{j=1}^k b_j^2/\lambda_j\right\}^{1/2}$. Then

$$\lambda P^tD^{-1}V^tCVD^{-1}P = \begin{pmatrix} n\lambda - b_0 & -\gamma \\ -\gamma & 1 \end{pmatrix} \oplus I_{k-1} \oplus 0_{n-k-1},$$

which is positive semidefinite if and only if $\lambda \geq \left(b_0 + \sum_{j=1}^k b_k^2/\lambda_j\right)/n$. It follows that $\lambda C = \lambda ee^t - A$ is positive semidefinite and C is a correlation matrix whenever $\lambda \geq \left(b_0 + \sum_{j=1}^k b_k^2/\lambda_j\right)/n$.

By the argument in the preceding paragraph, we see that whenever

$$A = (\|x_i - x_j\|^2) = (\|x_i\|^2 + \|x_j\|^2 - 2x_i^tx_j) = \lambda\left(ee^t - (x_i^tx_j/\|x_i\|\|x_j\|)\right)$$

with $r = \|x_1\| = \cdots = \|x_n\|$, then $\lambda = 2r^2 \geq \left(b_0 + \sum_{j=1}^k b_k^2/\lambda_j\right)/n$. The last assertion follows.

(h) ⇔ (d). The equivalence of (h) and (d) is clear.

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(h) ⇔ (e). Let L denote the leading $(k+1) \times (k+1)$ principal submatrix of V^tAV. Because $\lambda_1, \ldots, \lambda_k > 0$, L has at least k negative eigenvalues. But $\text{trace}(L) = \text{trace}(V^tAV) = \text{trace}(A) = 0$, so $b_0 > 0$ and L must have a positive eigenvalue. Thus, $\text{rank}(L) = k+1$ and $\text{rank}(A) = \text{rank}(V^tAV) \geq k+1$. It is obvious from the form of (3.1) that $\text{rank}(A) = \text{rank}(V^tAV) > k+1$ if and only if some $b_i \neq 0$, $i \in \{k+1, \ldots, n-1\}$.

(h) ⇔ (f). Let V be the orthogonal matrix in (h). Then that $e^tw = 1$ if and only if $V^tw = (1, w_2, \ldots, w_n)^t$ for some $w_2, \ldots, w_n \in \mathbb{R}$. So, (f) holds if and only if $b_{k+1} = \cdots = b_n = 0$.

(d) ⇔ (g). It is easy to show that (d) and (g) are equivalent.

(h) ⇔ (c). Using the matrix representation in (h), we see that the intersection of the range space of A and the null space of $(I - ee^t/n)A(I - ee^t/n)$ contains the vector e. It has dimension one if and only if $b_{k+1} = \cdots = b_n = 0$.

(b) ⇒ (i). Note that for $\lambda \geq 0$ and correlation matrix C, that $-\lambda y^tCy \leq 0$. It follows that $\sum a_{ij}y_iy_j = y^tAy = \lambda y^tee^ty - \lambda y^tCy \leq \lambda(\sum y_i)^2$. Thus, condition (i) holds with $M = \lambda$.

(i) ⇒ (f). If there exists an M such that $\sum\limits_{i,j=1}^{n} a_{ij}y_iy_j \leq M \left(\sum\limits_{i=1}^{n} x_i\right)^2$ for all $y \in \mathbb{R}^n$, then restrict y to those values such that $\sum y_i = e^ty = 1$. Then $y^tAy \leq M < \infty$ for all such y. □

The equivalence of (a) and (e) was observed by Gower [7, Theorem 6]. The equivalence of (a) and (d) of Theorem 3.1 and the last assertion were obtained in [12, Theorem 3.1 and Corollary 3.1].

Alfakih and Wolkowicz [1, Theorem 3.3] used Gale transforms to characterize those ESD matrices that can be represented as $A = \lambda(ee^t - C)$. In particular, they state condition (h) as $AZ = 0$, where Z is a *Gale matrix* associated with A. If $k = n-1$, then $Z = (0, \ldots, 0)^t$ and $AZ = 0$, while (h) is vacuously true. If $k < n-1$, then let $Z = (u_{k+1} \cdots u_{n-1})Q$, where $u_1, \ldots, u_{n-1}$ are the columns of U and Q is nonsingular. Then $U^tAZ = 0$ and, because the rows of U^t form a basis for $e^{\perp}$, the columns of AZ lie in the span of e. Hence, $AZ = 0$ if and only if $(b_{k+1}, \ldots, b_{n-1})^t = e^tAZ = 0$.

Using condition (b), one can deduce that $\text{CESD}(n)$ is a convex cone. Note that it is highly non-trivial to prove that $\text{CESD}(n)$ is a convex cone using the definition.

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The next result is noted in [5, p. 535], as a corollary of an elegant but complicated general theory of cuts and metrics. Here we provide a direct proof and some refinements.

THEOREM 3.2. *The set* $\mathrm{CESD}(n)$ *is dense in* $\mathrm{ESD}(n)$*, i.e.,* $\mathrm{ESD}(n)$ *equals the closure of* $\mathrm{CESD}(n)$*.*

Proof. Suppose $A \in \mathrm{ESD}(n)$ has rank m. If A has embedding dimension $m-1$, then $A \in \mathrm{CESD}(n)$. Otherwise, let $A = (\|x_i - x_j\|^2)$ such that $x_1, \ldots, x_n \in \mathbb{R}^{m-2}$ so that $\sum_{j=1}^n x_j = 0$. Let X be the $(m-2) \times n$ matrix with $x_1, \ldots, x_n$ as column. Then there is an $(n-m+1) \times n$ matrix so that the columns of X^t and Y^t together form an orthonormal basis for $e^\perp$. For $\varepsilon > 0$, let Z_ε be the $(n-1) \times n$ matrix with the top $m-2$ rows from the matrix X, and the bottom $n-m+1$ rows from the matrix εY. Let $y_1, \ldots, y_n \in \mathbb{R}^{n-m+1}$ be the column of Y. Then

$$A_\varepsilon = \kappa(Z_\varepsilon^t Z_\varepsilon) = (\|x_i - x_j\|^2) + \varepsilon^2(\|y_i - y_j\|^2)$$

has embedding dimension $n-1$, and hence belongs to $\mathrm{CESD}(n)$. Evidently, A_ε approaches A as $\varepsilon \to 0$. ∎

4. Linear preservers. In this section, we study linear maps leaving invariant the cones of $\mathrm{ESD}(n)$ and $\mathrm{CESD}(n)$. Actually, using the correspondence between positive semidefinite matrices, ESD matrices and CESD matrices, we can obtain better results. We begin by characterizing the linear operators that preserve PSD matrices with specific ranks.

THEOREM 4.1. *Let* $K = \{k_1, \ldots, k_m\} \neq \{0\}$ *be such that* $0 \le k_1 < \cdots < k_m \le n-1$*. Let*

$$\mathcal{C} = \{C \in \mathrm{PSD}(n-1) : \mathrm{rank}(C) \in K\}. \tag{4.1}$$

Then a linear operator $T : \mathbf{S}_{n-1} \to \mathbf{S}_{n-1}$ *satisfies* $T(\mathcal{C}) = \mathcal{C}$ *if and only if there exists an invertible matrix* R *such that*

$$T(C) = R^t C R \qquad \text{for all } C \in \mathbf{S}_{n-1}.$$

Proof. If $T(C) = R^t C R$ with R invertible, then it follows from Sylvester's Law of Inertia that $T(C)$ has the same number of positive, negative and zero eigenvalues, i.e., is PSD of the same rank. Thus, we see that $T(\mathcal{C}) = \mathcal{C}$. It remains to establish the converse. Let

$$\mathcal{C}_j = \{C \in \mathrm{PSD}(n-1) : \mathrm{rank}(C) = j\} \qquad \text{and} \qquad \hat{\mathcal{C}}_k = \bigcup_{j=0}^{k} \mathcal{C}_j.$$

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We claim that $\hat{\mathcal{C}}_k = \mathrm{cl}(\mathcal{C}_k)$, the closure of $\mathcal{C}_k$.

Because $\mathcal{C}_k \subseteq \hat{\mathcal{C}}_k$ and $\hat{\mathcal{C}}_k$ is closed, we see that $\mathrm{cl}(\mathcal{C}_k) \subseteq \hat{\mathcal{C}}_k$. If $C \in \mathcal{C}_k$, then obviously $C \in \mathrm{cl}(\mathcal{C}_k)$. If $C \in \mathcal{C}_j$ for $j < k$, then write $C = Y_j^t Y_j$ for a $j \times (n-1)$ matrix Y_j. Let Y_{k-j} be any $(k-j) \times (n-1)$ matrix such that $(Y_j^t | Y_{k-j}^t)$ has rank k, let $c = 1/\|Y_{k-j}^t Y_{k-j}\|$, and let $C_i = Y_j^t Y_j + (c/i) Y_{k-j}^t Y_{k-j}$. Then $C_i \in \mathcal{C}_k$ and $\|C_i - C\| = 1/i \to 0$ as $i \to \infty$, so each $C \in \hat{\mathcal{C}}_k$ is the limit point of a sequence in $\hat{\mathcal{C}}_k$. This proves that $\hat{\mathcal{C}}_k \subseteq \mathrm{cl}(\mathcal{C}_k)$. It also demonstrates that $\mathrm{int}(\hat{\mathcal{C}}_k)$, the relative interior of $\hat{\mathcal{C}}_k$, is contained in $\mathcal{C}_k$. Because $\mathcal{C}_k \subseteq \hat{\mathcal{C}}_k$ and $\hat{\mathcal{C}}_k$ is closed, $\mathrm{cl}(\mathcal{C}_k) \subseteq \hat{\mathcal{C}}_k$. We have also shown that because $\mathcal{C}_k$ is open in $\hat{\mathcal{C}}_k$, $\mathrm{int}(\hat{\mathcal{C}}_k) = \mathcal{C}_k$.

Now suppose that $T(\mathcal{C}) = \mathcal{C}$. Because T is continuous,

$$T\left(\hat{\mathcal{C}}_{k_m}\right) = T\left(\mathrm{cl}\left(\mathcal{C}\right)\right) = \mathrm{cl}\left(\mathcal{C}\right) = \hat{\mathcal{C}}_{k_m}. \tag{4.2}$$

Because T is linear,

$$T\left(\mathcal{C}_{k_m}\right) = T\left(\mathrm{int}\left(\hat{\mathcal{C}}_{k_m}\right)\right) = \mathrm{int}\left(\hat{\mathcal{C}}_{k_m}\right) = \mathcal{C}_{k_m}. \tag{4.3}$$

From (4.3) and (4.2), we obtain

$$T\left(\hat{\mathcal{C}}_{k_m-1}\right) = T\left(\hat{\mathcal{C}}_{k_m} - \mathcal{C}_{k_m}\right) = T\left(\hat{\mathcal{C}}_{k_m}\right) - T\left(\mathcal{C}_{k_m}\right) = \hat{\mathcal{C}}_{k_m} - \mathcal{C}_{k_m} = \hat{\mathcal{C}}_{k_m-1}.$$

We continue to "peel the onion" in this manner, i.e., using an inductive argument, concluding that $T(\mathcal{C}_1) = \mathcal{C}_1$. It then follows from Theorem 3 in [8] that T is of the form $T(C) = \pm R^t C R$. Because C and $T(C)$ are positive semidefinite, we conclude that $T(C) = R^t C R$. □

Next we set $w = e$ and characterize the linear operators that preserve subsets of $G_e(n)$ containing matrices with specific ranks.

THEOREM 4.2. *Let* $K = \{k_1, \ldots, k_m\} \neq \{0\}$ *be such that* $0 \leq k_1 < \cdots < k_m \leq n-1$. *Let*

$$\mathcal{B} = \left\{B \in G_e(n) : \mathrm{rank}(B) \in K\right\}. \tag{4.4}$$

Then a linear operator $T : [G_e(n)] \to [G_e(n)]$ *satisfies* $T(\mathcal{B}) = \mathcal{B}$ *if and only if there exists an* $n \times n$ *matrix* Q, *with rank*$(Q) = n-1$ *and* $Qe = Q^t e = 0$, *such that*

$$T(B) = Q^t B Q \qquad \textit{for all } B \in [G_e(n)].$$

Proof. Fix $w = e$ and U, any $n \times (n-1)$ matrix for which $(\frac{e}{\sqrt{n}}|U)$ is orthogonal. Then $W = U^t(I - \frac{ee^t}{n}) = U^t$, so $\psi_u(B) = U^t B U$ and $\phi_u(C) = W^t C W = U C U^t$.

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Let $\mathcal{C} = \psi_u(\mathcal{B})$, in which case $\mathcal{B} = \phi_u(\mathcal{C})$. Then $T(\mathcal{B}) = \mathcal{B}$ if and only if $T\circ\phi_u(\mathcal{C}) = \phi_u(\mathcal{C})$ if and only if $\psi_u \circ T \circ \phi_u(\mathcal{C}) = \mathcal{C}$. Because ψ_u and ϕ_u preserve rank, $\mathcal{C} \subseteq \mathrm{PSD}(n-1)$ is a set of the form (4.1); hence, it follows from Theorem 4.1 that $T(\mathcal{B}) = \mathcal{B}$ if and only if there exists an invertible matrix R such that $\psi_u \circ T \circ \phi_u(C) = R^tCR$.

Suppose that there exists an $(n-1)\times(n-1)$ invertible matrix R such that $\psi_u \circ T \circ \phi_u(C) = R^tCR$. Let $Q = URU^t$. Then $\mathrm{rank}(Q) = n-1$, $Qe = Q^te = 0$, and

$$\begin{aligned} T(B) &= \phi_u \circ \psi_u \circ T \circ \phi_u \circ \psi_u(B) = \phi_u \circ \psi_u \circ T \circ \phi_u \left(U^tBU\right) \\ &= \phi_u \left(R^tU^tBUR\right) = UR^tU^tBURU^t = Q^tBQ. \end{aligned}$$

Conversely, suppose that there exists an $n\times n$ matrix Q such that $\mathrm{rank}(Q) = n-1$, $Qe = Q^te = 0$, and $T(B) = Q^tBQ$. Let $R = U^tQU$. Then R is invertible and

$$\psi_u \circ T \circ \phi_u(C) = \psi_u \circ T \left(UCU^t\right) = \psi_u \left(Q^tUCU^tQ\right) = U^tQ^tUCU^tQU = R^tCR. \qquad \square$$

Now, we characterize the linear operators that preserve matrices in $\mathrm{ESD}(n)$ with specific embedding dimensions. Let $\dim(A)$ denote the embedding dimension of $A \in \mathrm{ESD}(n)$.

THEOREM 4.3. *Let* $K = \{k_1, \ldots, k_m\} \neq \{0\}$ *be such that* $0 \le k_1 < \cdots < k_m \le n-1$. *Let*

$$\mathcal{A} = \{A \in \mathrm{ESD}(n) : \dim(A) \in K\}.$$

Then a linear operator $T : [\mathrm{ESD}(n)] \to [\mathrm{ESD}(n)]$ *satisfies* $T(\mathcal{A}) = \mathcal{A}$ *if and only if there exists an* $n \times n$ *matrix* Q*, with rank*$(Q) = n-1$ *and* $Qe = Q^te = 0$*, such that*

$$T(A) = -\kappa(Q^tAQ)/2 \qquad \textit{for all } A \in [\mathrm{ESD}(n)].$$

Proof. Let $\mathcal{B} = \tau_e(\mathcal{A})$, in which case $\mathcal{A} = \kappa(\mathcal{B})$. Then $T(\mathcal{A}) = \mathcal{A}$ if and only if $T \circ \kappa(\mathcal{B}) = \kappa(\mathcal{B})$ if and only if $\tau_e \circ T \circ \kappa(\mathcal{B}) = \mathcal{B}$. Because of the equivalence of conditions (a) and (b) in Theorem 2.1, $\mathcal{B} \subseteq G_e(n)$ is a set of the form (4.4); hence, it follows from Theorem 4.2 that $T(\mathcal{A}) = \mathcal{A}$ if and only if there exists an $n \times n$ matrix Q, with $\mathrm{rank}(Q) = n-1$ and $Qe = Q^te = 0$, such that

$$\tau_e \circ T \circ \kappa(B) = Q^tBQ. \tag{4.5}$$

Now we apply κ to both sides of (4.5), obtaining

$$\begin{aligned} T(A) &= T \circ \kappa(B) = \kappa\left(Q^tBQ\right) = \kappa\left(Q^t\tau_e(A)Q\right) \\ &= -\frac{1}{2}\kappa\left(Q^t\left(I - \frac{ee^t}{n}\right)A\left(I - \frac{ee^t}{n}\right)Q\right) = -\frac{1}{2}\kappa\left(Q^tAQ\right). \qquad \square \end{aligned}$$

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By the fact that the closure of CESD(n) equals ESD(n), we have the following.

THEOREM 4.4. *A linear operator* $T : [\text{CESD}(n)] \to [\text{CESD}(n)]$ *satisfies*

$$T(\text{CESD}(n)) = \text{CESD}(n)$$

if and only if there exists an $n \times n$ *matrix* Q*, with rank*$(Q) = n-1$ *and* $Qe = Q^t e = 0$*, such that*

$$T(A) = -\kappa(Q^t AQ)/2 \qquad \textit{for all } A \in [\text{CESD}(n)].$$

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